Neutrino Factory and Muon Collider Collaboration Meeting

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Numerical Simulation of Hg-Jet Target

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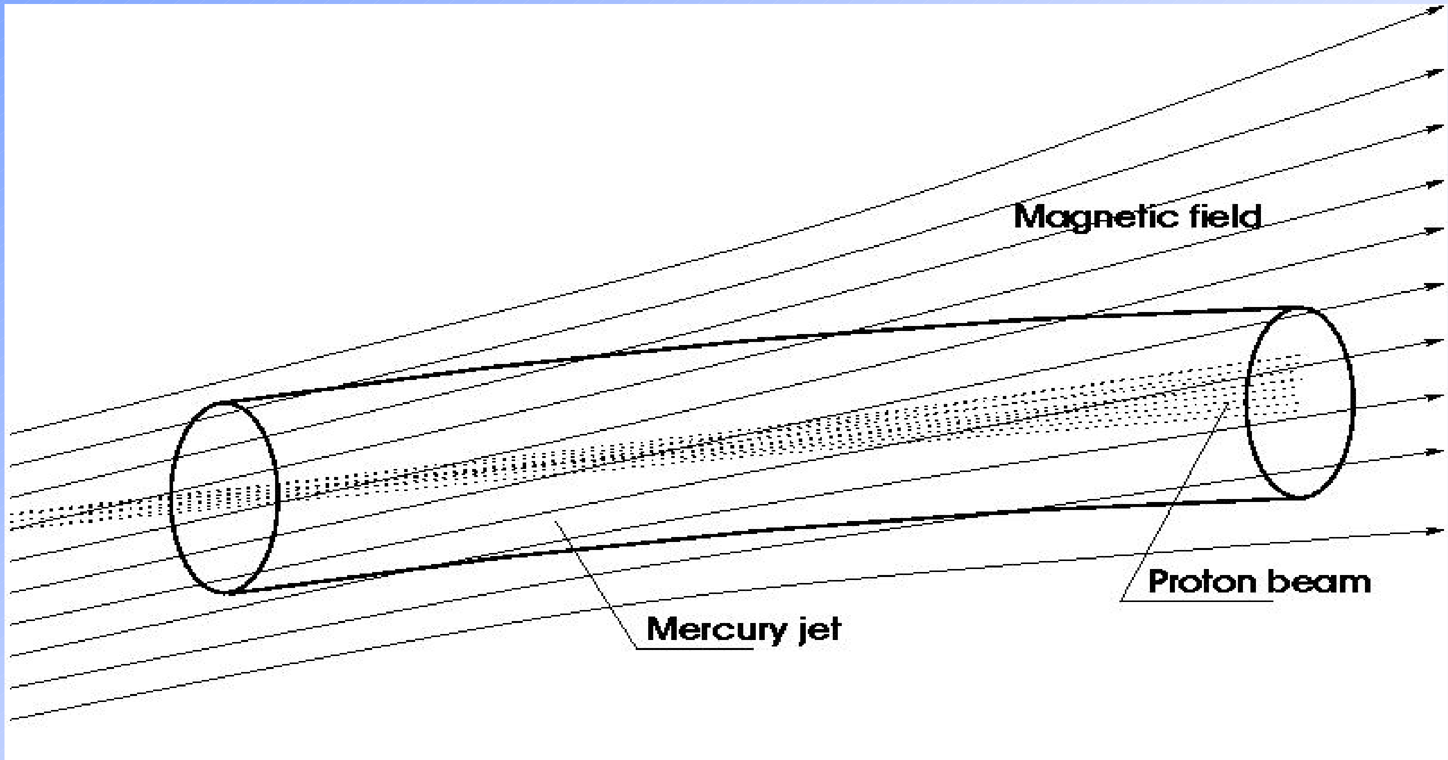
Talk outline

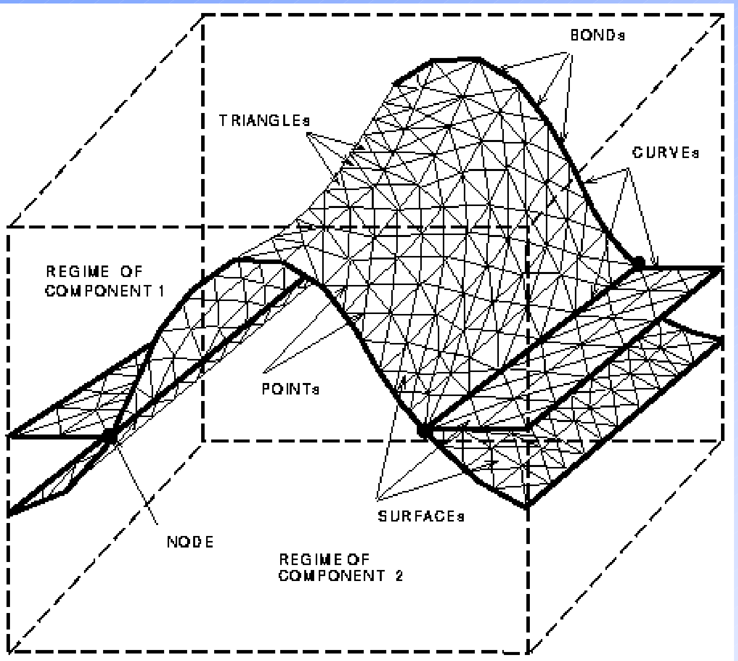
- FronTier-MHD code: theory and implementation.
- Brief overview of MHD simulations
- Equations of state appropriate for the target modeling
- Modeling of the equation of state with phase transition (Riemann problem for such EOS)
- Numerical simulation of the mercury jet interacting with proton pulses.
- Future research.

Schematic of the Muon Collider Target



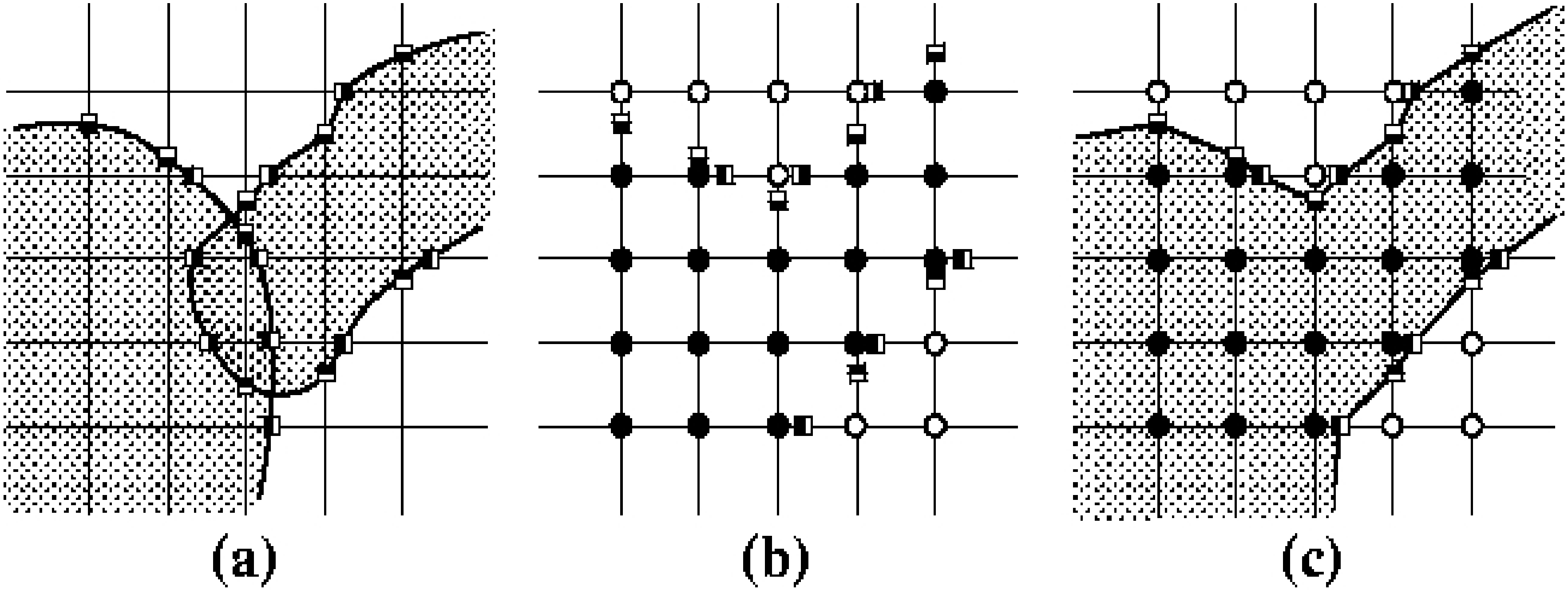
3D FronTier Structures

Interfaces model different types of discontinuities in a medium such as shock waves in gas dynamics, boundaries between fluid-gas states, different fluids or their phases in fluid dynamics, component boundaries in solid dynamics etc.

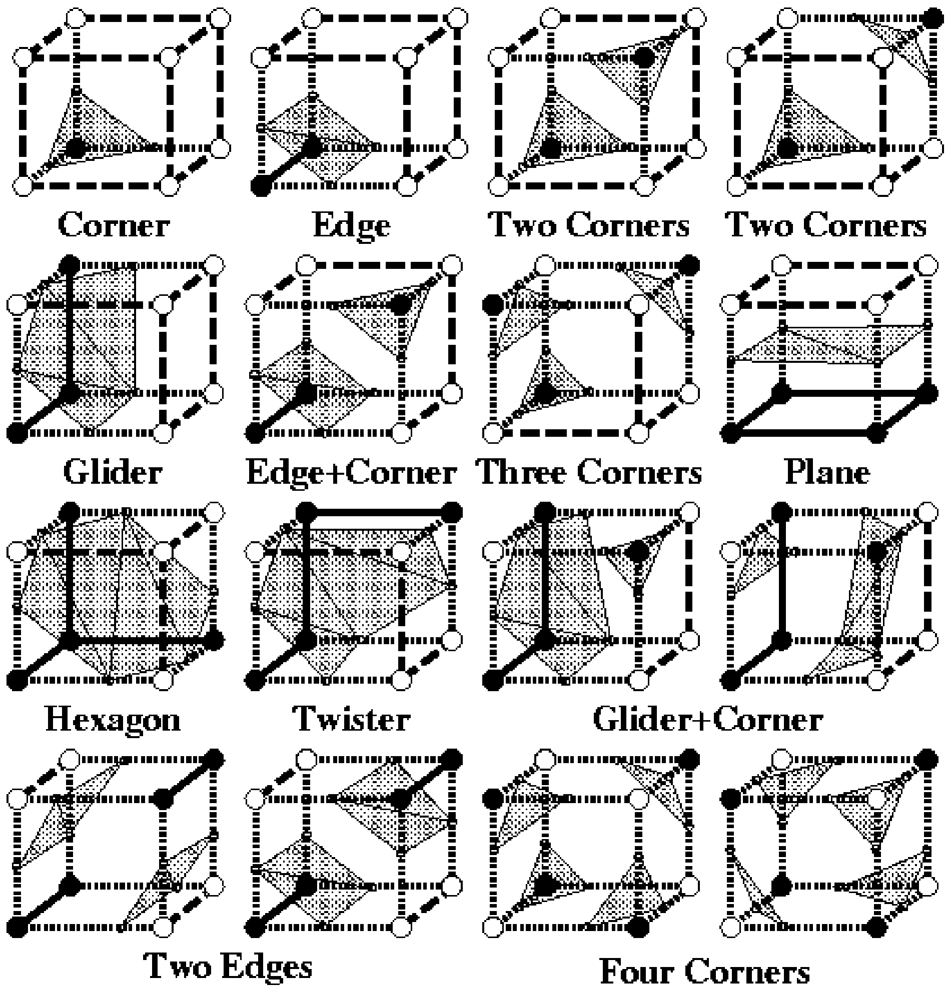


Front tracking represents interfaces as lower dimensional meshes moving through a volume filling grid. The traditional volume filling finite difference grid supports smooth solutions located in the region between interfaces and the lower dimensional grid or interface defines the location of the discontinuity and the jump in the solution variables across it.

Resolving interface tangling by using the grid based method



Greed based reconstruction of the interface



We reconstruct the interface using micro-topology within each rectangular grid cell. There are 256 possible configurations for the crossings of the cell edge by the interface. Through elementary operations of rotation, reflection and separation these can be reduced to the 16 cases shown on the left.

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The *FronTier* code: capabilities of the interior solvers

FronTier uses high resolution methods for the interior hyperbolic solvers such as Lax-Wendroff, Godunov and MUSCL and the following Riemann solvers:

- Exact Riemann solver
- Colella-Glaz approximate Riemann solver
- Linear US/UP fit (Dukowicz) Riemann solver
- Gamma law fit

FronTier uses realistic models for the equation of state:

- Polytropic Equation of State
- Stiffened Polytropic Equation of State
- Gruneisen Equation of State
- SESAME Tabular Equation of State

The system of equation of compressible magnetohydrodynamics

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u})$$

$$\rho\left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla\right)\mathbf{u} = -\nabla P + \rho \mathbf{X} + \frac{1}{c}(\mathbf{J} \times \mathbf{B})$$

$$\rho\left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla\right)U = -P\nabla \cdot \mathbf{u} + \frac{1}{\sigma}\mathbf{J}^2 - \frac{1}{c}\mathbf{u} \cdot (\mathbf{J} \times \mathbf{B})$$

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{u} \times \mathbf{B}) - \nabla \times \left(\frac{c^2}{4\pi\sigma}\nabla \times \mathbf{B}\right)$$

$$\nabla \cdot \mathbf{B} = 0$$

The interface condition

Interface conditions for the normal and tangential components of the magnetic field

$$\mathbf{n}\cdot\left(\mathbf{B}_2-\mathbf{B}_1\right)=0,$$

$$\mathbf{n}\times\left(\mathbf{H}_2-\mathbf{H}_1\right)=\frac{4\pi}{c}\mathbf{K},$$

where $\mathbf{B}=\mu\mathbf{H}.$

Approximations:
I. General case

General approach: the magnetic field is not constant in time.

Time scales: acoustic waves time scale = 7 microseconds;
magnetic diffusion time scale = 33 microseconds
Alfven waves time scale = 70 microseconds

Approximations:
II. Constant in time magnetic field

The magnetic field is constant in time. The distribution of currents can be found by solving Poisson's equation:

$$\mathbf{J} = \sigma\left(-\nabla\phi + \frac{1}{c}\mathbf{u}\times\mathbf{B}\right)$$

$$\Delta\phi = \frac{1}{c}\nabla\cdot\left(\mathbf{u}\times\mathbf{B}\right),$$

$$\text{with}\quad \left.\frac{\partial\phi}{\partial\mathbf{n}}\right|_{\Gamma} = \frac{1}{c}(\mathbf{u}\times\mathbf{B})\cdot\mathbf{n}$$

Magnetohydrodynamics of Multi Fluid Systems: Numerical Approach

- The system of MHD equations contains the hyperbolic subsystem (the mass, momentum and energy conservation equations) and the parabolic (the magnetic field evolution equation) or elliptic (Poisson’s equation for the current density distribution) subsystems.

- The hyperbolic subsystem is solved on a finite difference grid in both domains separated by the free surface using FronTier's interface tracking numerical techniques. The evolution of the free fluid surface is obtained through the solution of the Riemann problem for compressible fluids.

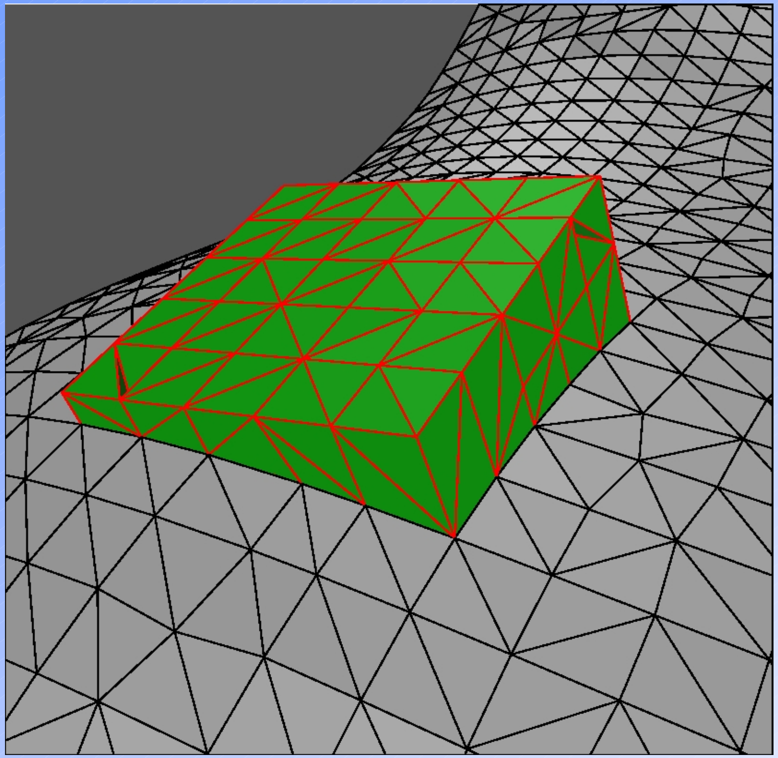
- The parabolic subsystem or elliptic subsystems is solved using a vector finite elements method based on Whitney elements. The grid is rebuilt at every time step and conformed to the evolving interface.

Finite element mesh generation with interface constraints: Point shift method.

1. Distortion of appropriate mesh blocks into irregular, convex hexahedra by shifting appropriate corner nodes to be coincident with the triangulated surface.
2. Appropriate redistribution of surface triangles to ensure that surface triangles are coplanar either with shifted hexahedra faces or "interior diagonal" planes.
3. Tetrahedralization of all (regular and irregular) grid blocks, creating and modifying a regularly indexed grid to provide a restricted optimized match to a triangulated tracked surface.

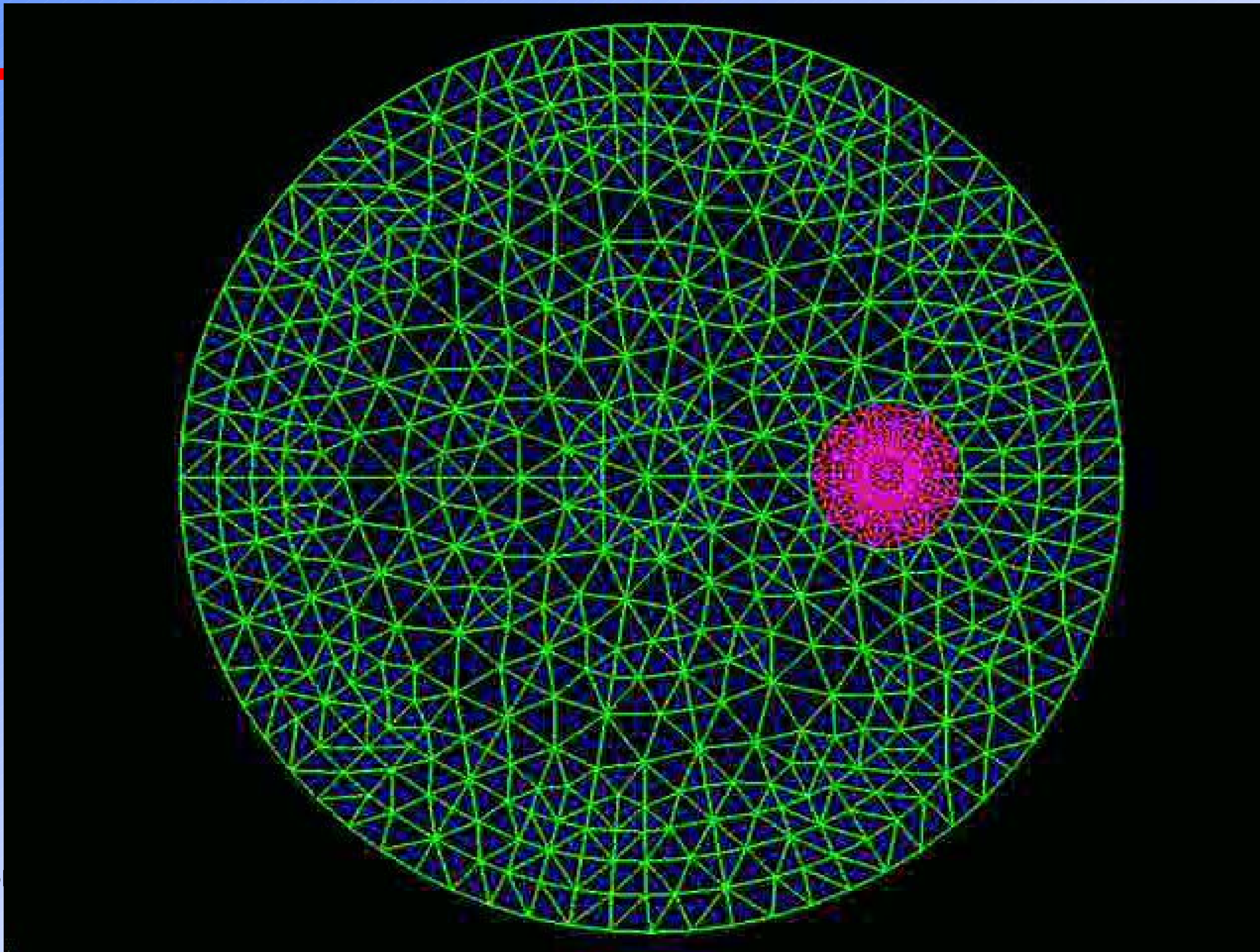
Advantages: preserves rectangular index structure.
Disadvantages: not robust (at present) in parallel.

Finite element mesh generation with interface constraints



Triangulated tracked surface and tetrahedralized hexahedra conforming to the surface. For clarity, only a limited number of hexahedra have been displayed.

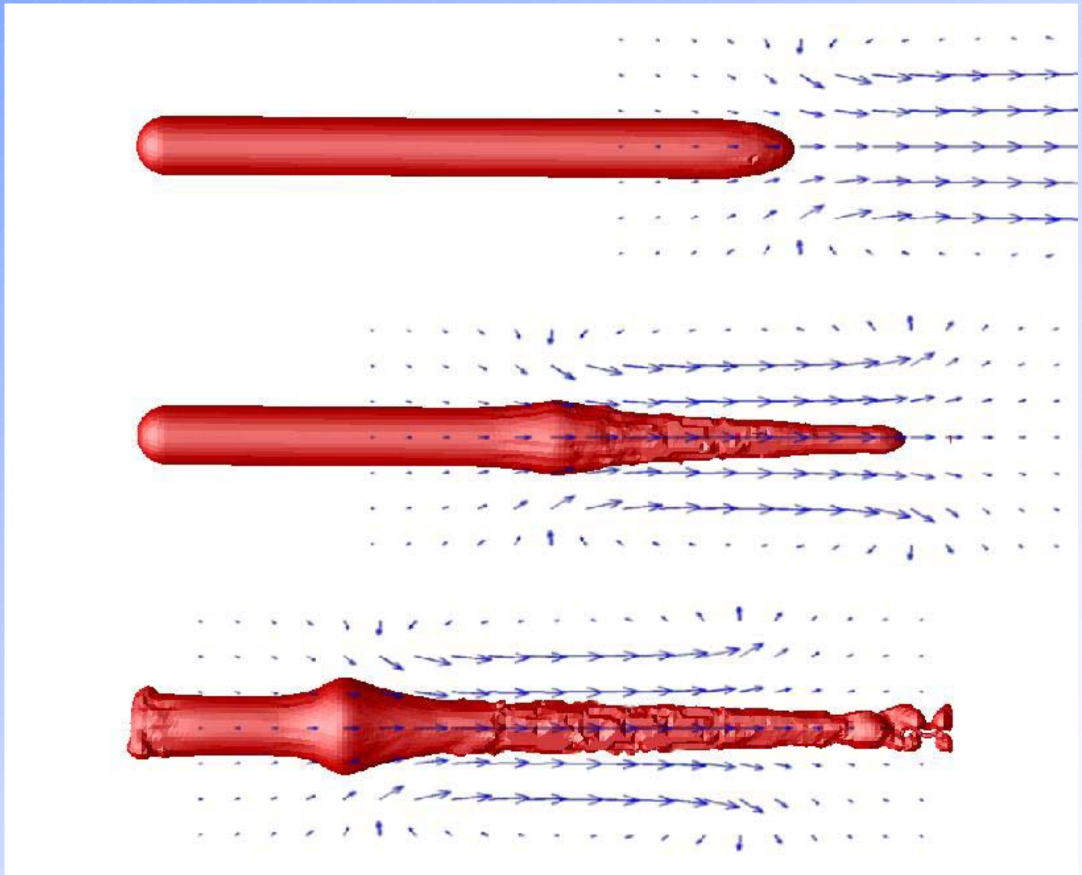
Dynamic finite element grid generation



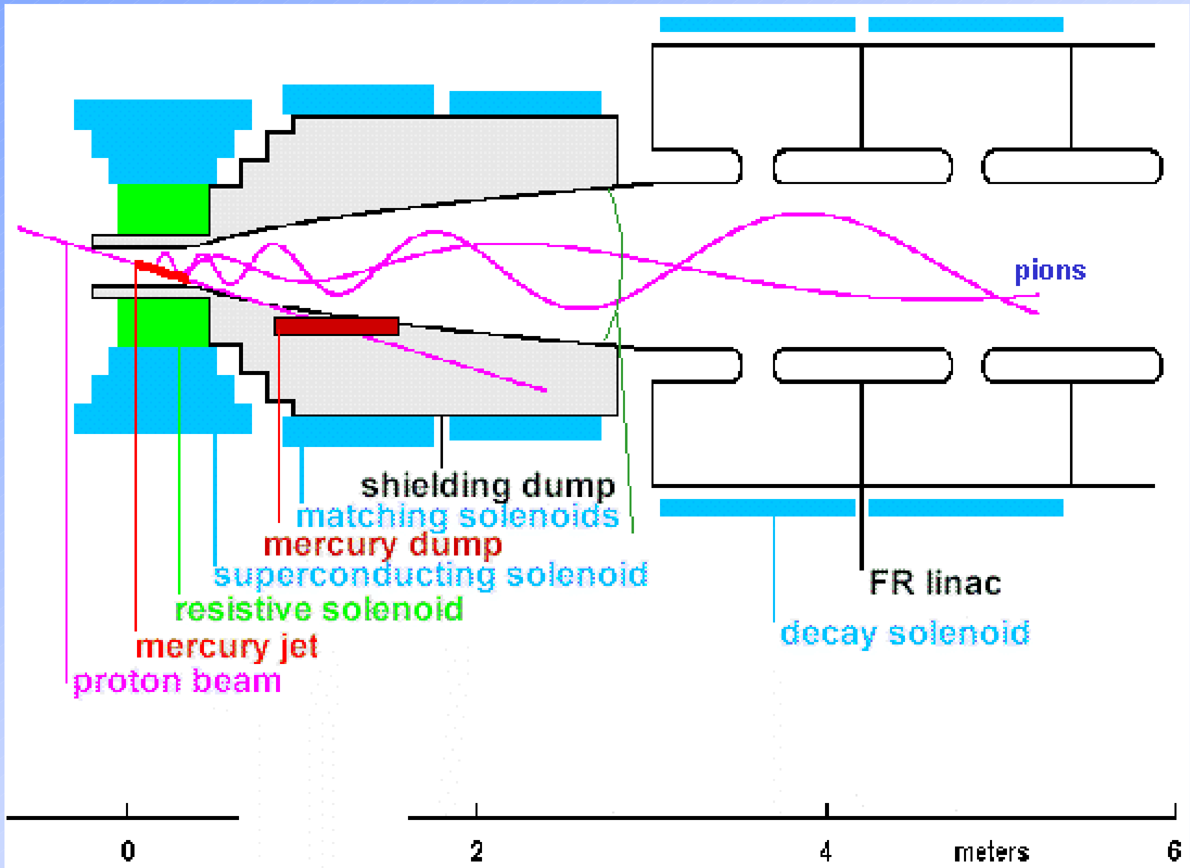
Previous Accomplishments:

Numerical Results

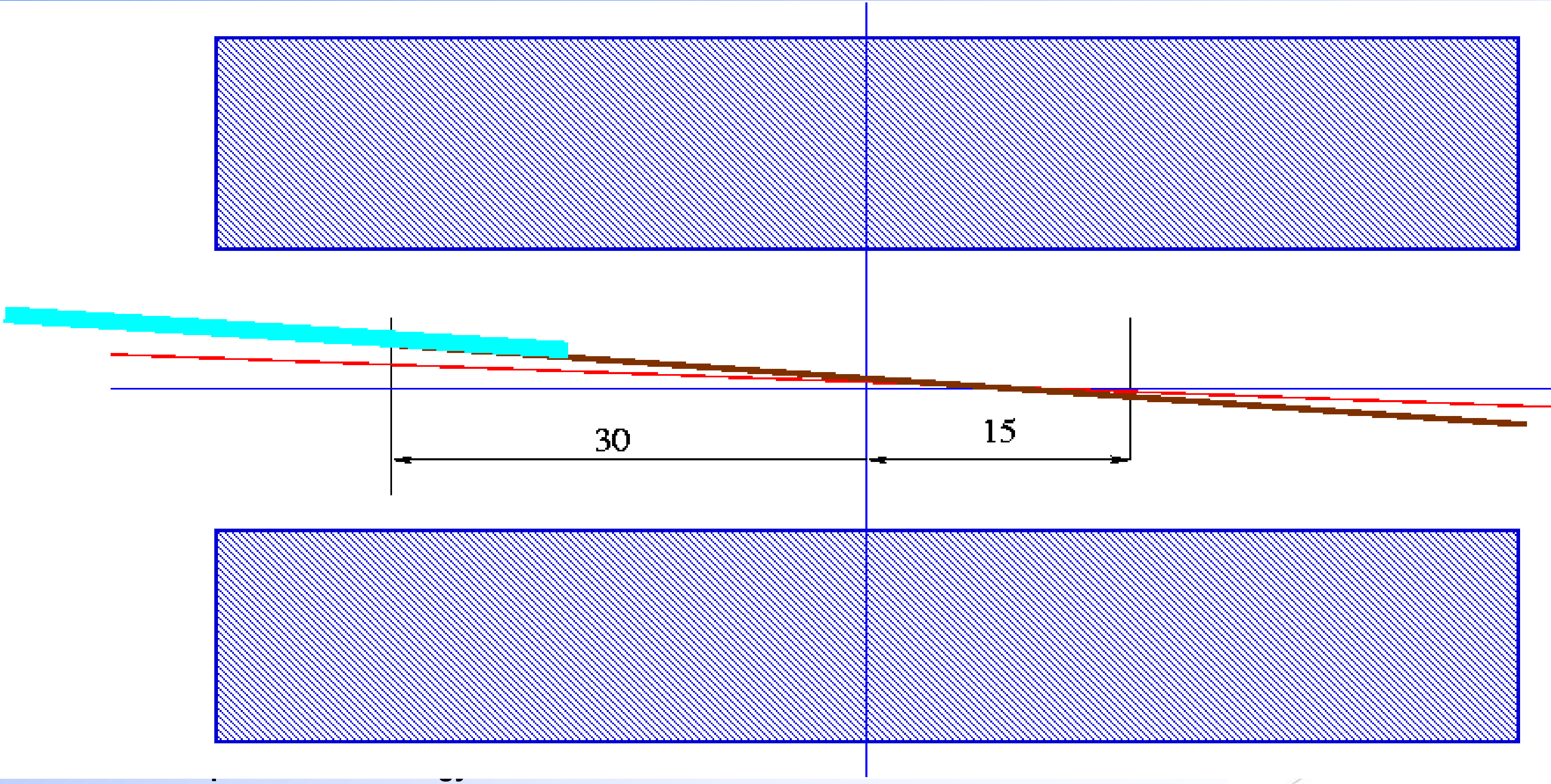
Liquid metal jet in 20 T solenoid



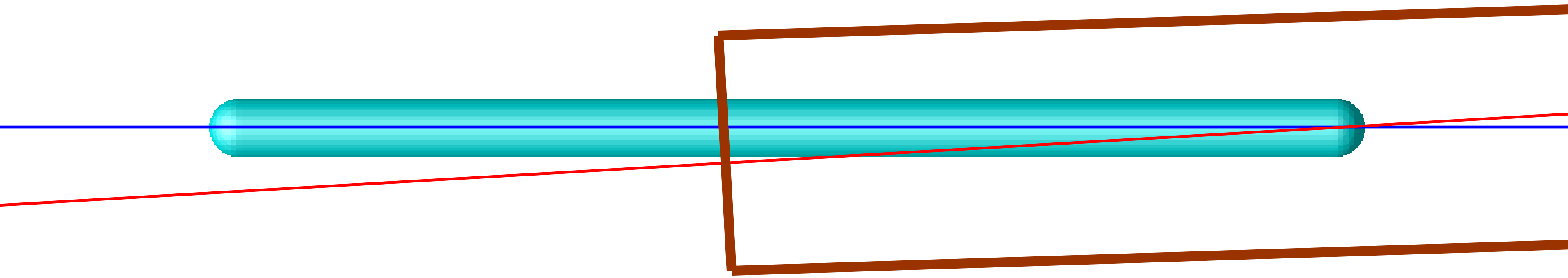
Schematic of the muon collider magnet system



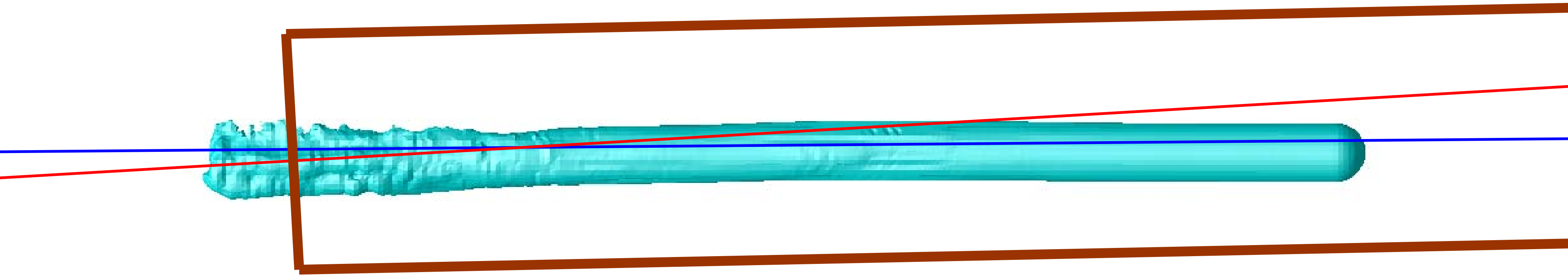
Mercury target in 20 T magnet



Mercury target in 20 T magnet



Mercury target in 20 T magnet



EOS models

- Equation of state for one phase liquid. Allows negative pressures (nonequilibrium thermodynamic)

- Isentropic two phase equation of state for cavitating liquid (equilibrium thermodynamics, no negative pressures)

- SESAME tabulated equation of state for mercury (does not allow phase transitions).

Equation of state

An EOS is a relation expressing the specific internal energy E of a material as a function of the entropy S and the specific volume V: $E(S,V)$.

The pressure P and temperature T are first derivatives of the energy E :

$$P(V,S) = -\left.\frac{\partial E}{\partial V}\right|_S, \qquad T(V,S) = \left.\frac{\partial E}{\partial S}\right|_V$$

in accordance with the second law of thermodynamics: $TdS = dE + PdV$.

The second derivatives of the internal energy are related to the adiabatic exponent γ, the Gruneisen coefficient Γ and the specific heat g.

Constraints

Thermodynamic constraints:

• $E = E(S,V)$ is continuously differentiable and piecewise twice continuously differentiable.

• $T \geq 0, \quad P \geq 0.$

• E is jointly convex as a function of V and S. This translates into the inequalities $g \geq 0, \quad \gamma \geq 0$ and $\gamma g \geq \Gamma^2$,

Or equivalently $C_V^{-1} \geq C_P^{-1} \geq 0$ and $K_S^{-1} \geq K_T^{-1} \geq 0.$

Asymptotic constraints:

- $P(V,S) \to \infty$ as $V \to 0.$
- $P(V,S) \to 0$ as $V \to \infty.$
- $E(V,S) \to \infty$ and $P(V,S) \to \infty$ as $S \to \infty.$

Analytical model: Isentropic EOS with phase transitions

• Gas (vapor) phase is described by the polytropic EOS reduced to an isentrope.

$$P = (\gamma_0 - 1)E\rho,$$

$$T = \frac{P}{R\rho},$$

$$S = (\log P - \gamma_0 \log \rho)\frac{R}{\gamma_0 - 1}.$$

Analytical model: Isentropic EOS with phase transitions

- Mixed phase is described as follows:

$$P(\rho) = P_l^{sat} + P_{vl}\log\left[\frac{\rho_v a_v^2\left(\rho_l + \alpha(\rho_v - \rho_l)\right)}{\rho_l\left(\rho_v a_v^2 - \alpha\left(\rho_v a_v^2 - \rho_l a_l^2\right)\right)}\right],$$

$$E(\rho) = \int_{\rho_v^{sat}}^{\rho} \frac{P}{\rho^2}\, d\xi,$$

where

$$P_{vl} = \frac{\rho_v a_v^2 \rho_l a_l^2 (\rho_v - \rho_l)}{\rho_v^2 a_v^2 - \rho_l^2 a_l^2},$$

and α is the void fraction: $\alpha = \dfrac{\rho - \rho_l}{\rho_v - \rho_l}.$

Analytical model: Isentropic EOS with phase transitions

- Liquid phase is described by the stiffened polytropic EOS:

$$P = (\gamma - 1)\rho(E + E_\infty) - \gamma P_\infty,$$

$$T = \frac{P + P_\infty}{R\rho},$$

$$S = \left(\log(P + P_\infty) - \gamma_0 \log\rho\right)\frac{R}{\gamma_0 - 1}.$$

SESAME tabular equation of state

■ The SESAME EOS is a tabular equation of state which gives the thermodynamic functions for a large number of materials, including gases, metals and minerals, in a computerized database.

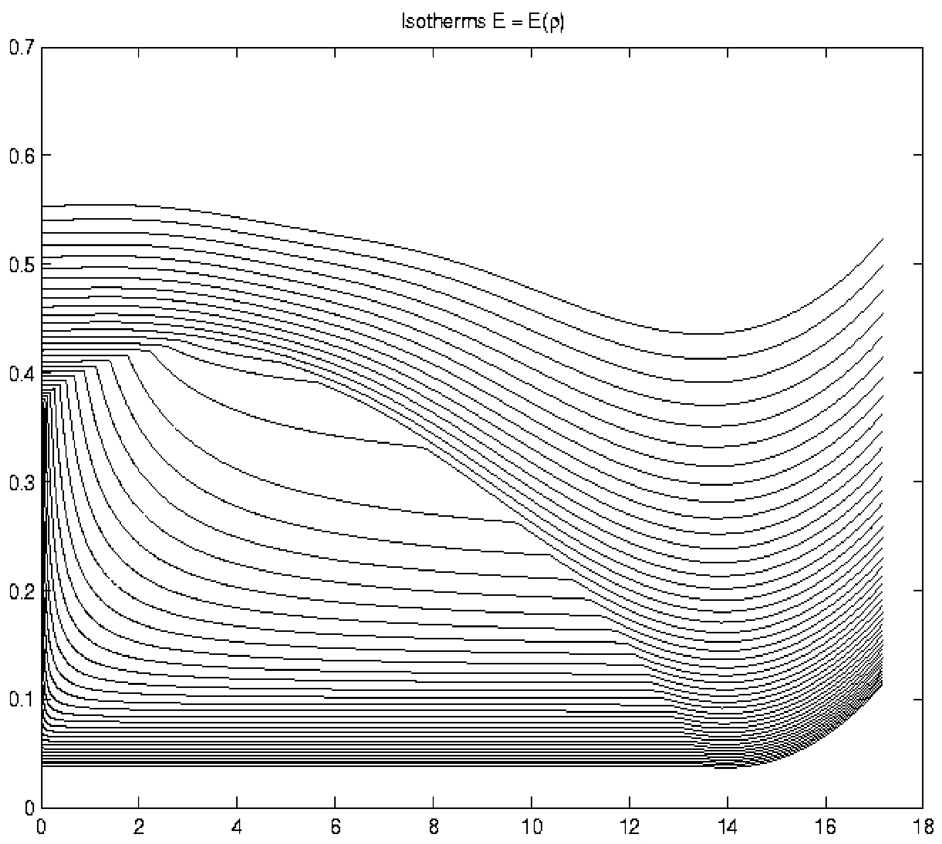
■ The SESAME EOS includes the following tables:

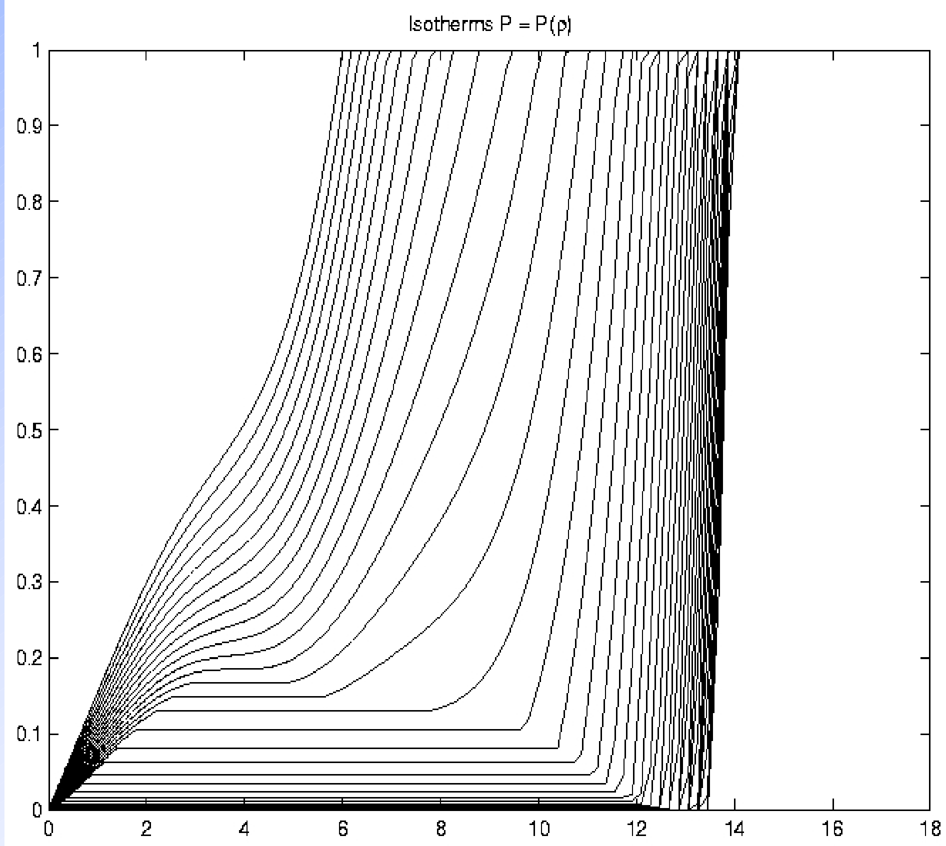
201 Tables. The 201 tables contains 5 floats which are the *atomic number, atomic weight, density, pressure* and *internal energy* at the normal conditions.

301 Tables. The 301 tables is a database for the *pressure, internal energy* and, in some cases, the *free energy* as functions of the *temperature* and *density*.

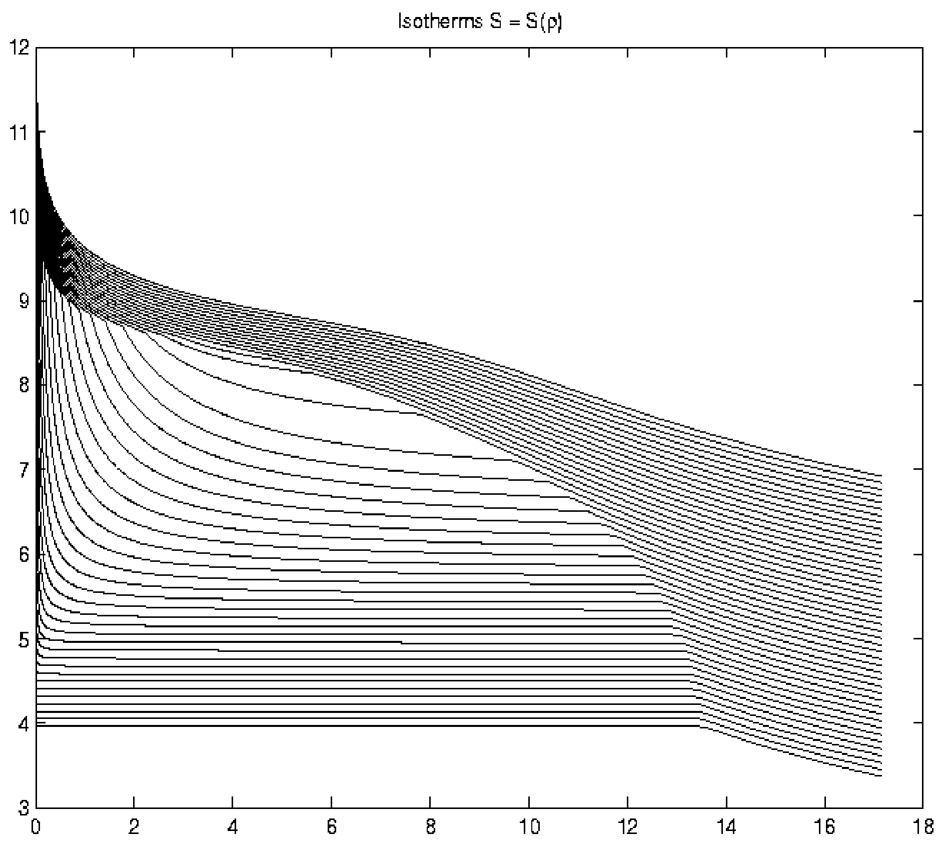
401 Tables. The 401 tables contain data for the thermodynamic functions at the liquid/vapor phase transition.

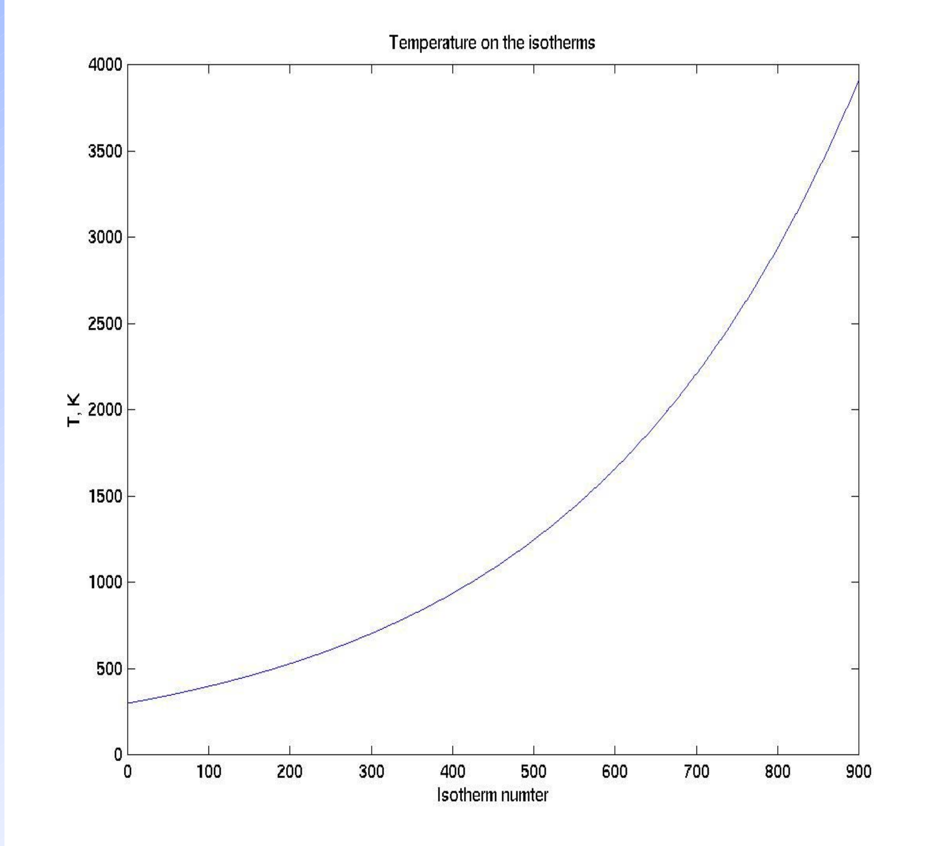
Thermodynamic properties of mercury, ANEOS data



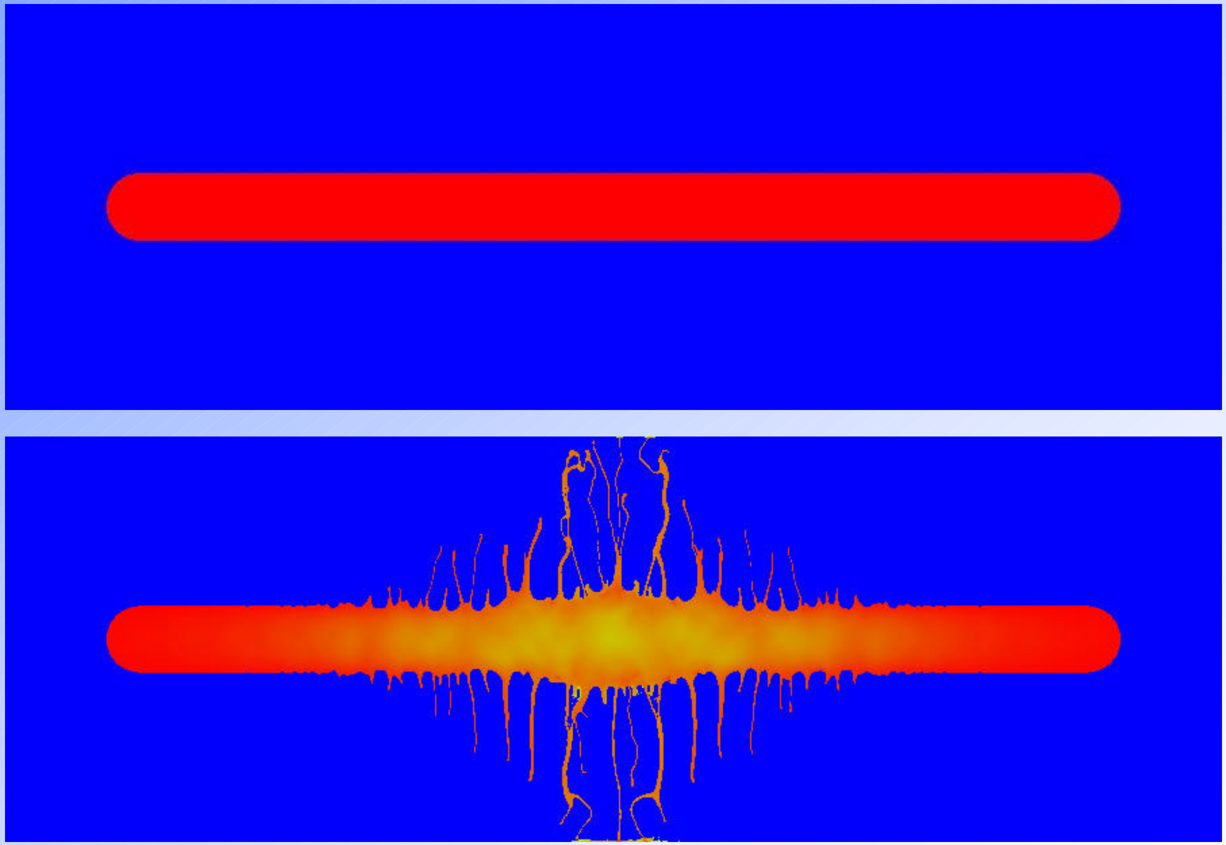


Thermodynamic properties of mercury, ANEOS data

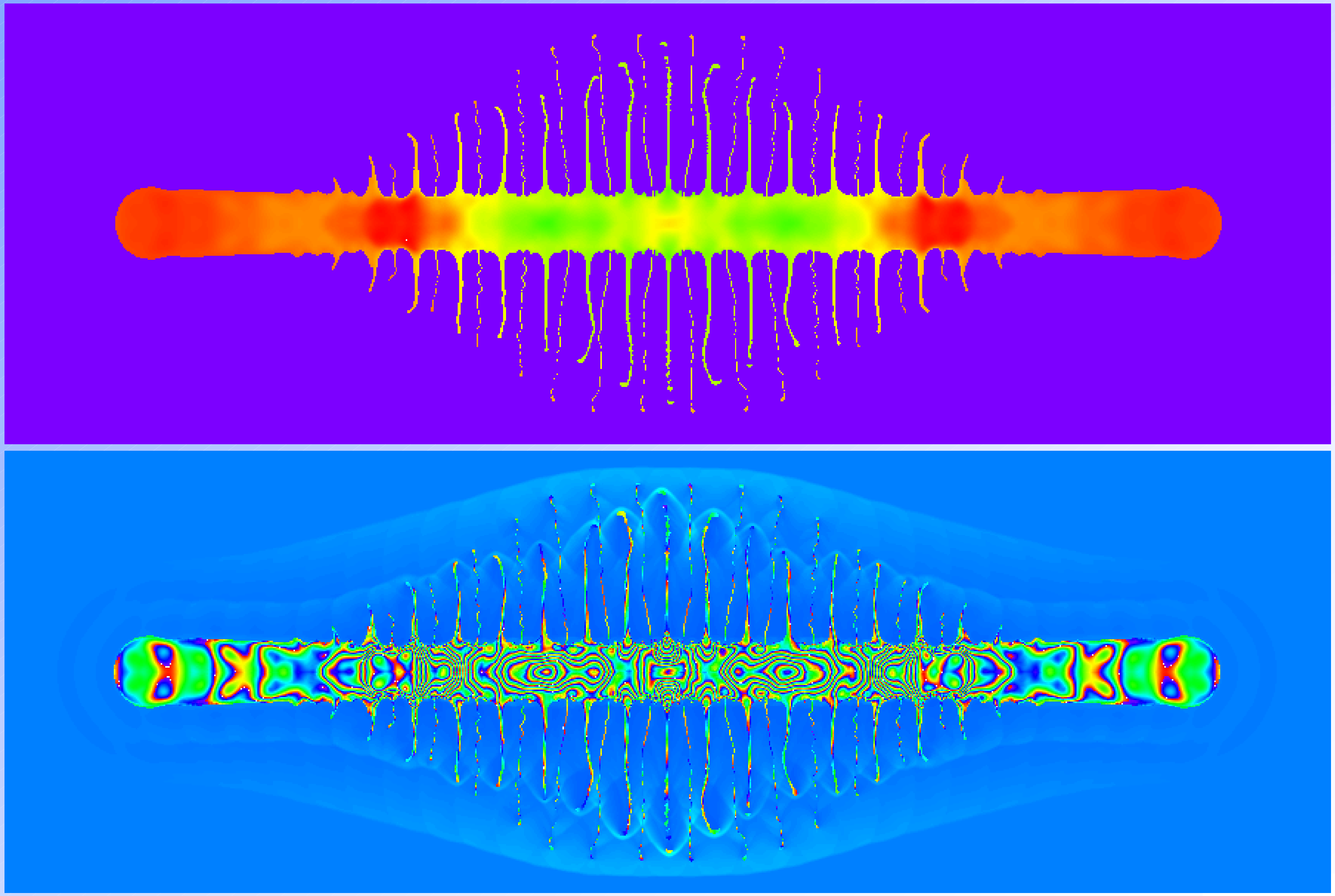




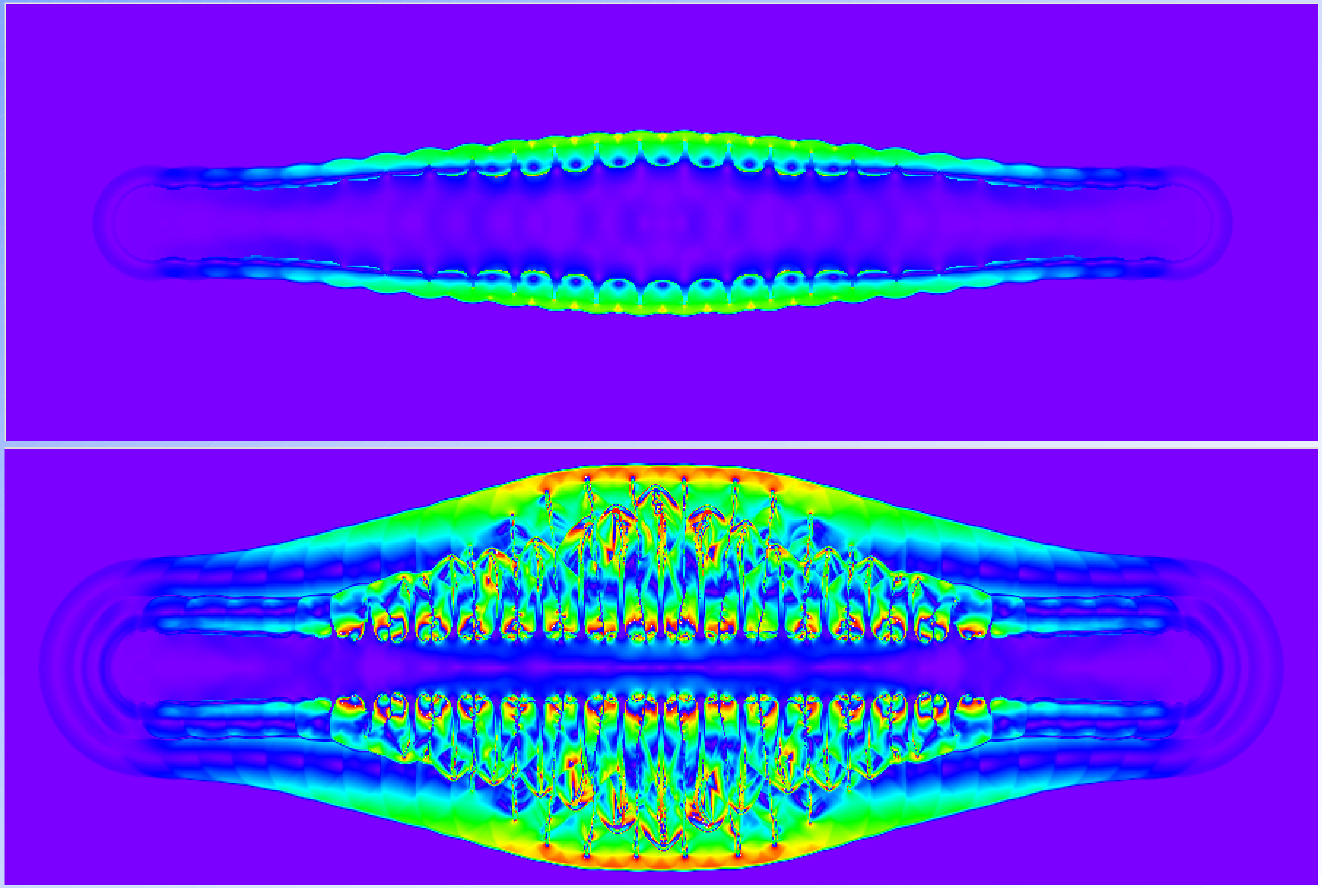
Simulation of the mercury jet – proton pulse interaction during 150 *mks* interval



Cavitation in the mercury jet



Distribution of the Mach number



Future Research

- Improve the robustness of the dynamic grid generator and implement new elliptic/hyperbolic solvers.
- Develop general analytic EOS for cavitating flows; nonequilibrium thermodynamics approach.
- Numerical simulation of nozzle effects.
- Further studies of liquid metal jets in magnetic fields.
- Numerical simulation of the mercury target interacting with a high energy proton beam in the presence of a strong magnetic field.
- Numerical simulation of turbulent jets.